

# Fermiology, Orbital order, Orbital Fluctuation and Cooper Pairing in Iron-based Superconductors

Fan Yang,<sup>1</sup> Fa Wang,<sup>2</sup> and Dung-Hai Lee<sup>3,4</sup>

<sup>1</sup>*School of Physics, Beijing Institute of Technology, Beijing 100081, P.R.China*

<sup>2</sup>*International Center for Quantum Materials and School of Physics, Peking University, Beijing 100871, China*

<sup>3</sup>*Department of Physics, University of California at Berkeley, Berkeley, CA 94720, USA*

<sup>4</sup>*Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*

We address two important issues that arise in recent studies of iron-based superconductivity. (1) Why are the  $T_c$  of  $A_x\text{Fe}_{2-y}\text{Se}_2$  and the single unit cell FeSe on  $\text{SrTiO}_3$  so high despite both only have electron pockets? (2) What (if any) are the effects of orbital order and orbital fluctuation on the Cooper pairing. Our conclusions are summarized in the third paragraph of the paper.

The discovery of  $A_x\text{Fe}_{2-y}\text{Se}_2$ [1] ( $T_c^{\text{max}} = 48\text{K}$ , under pressure[2]) and single unit cell FeSe on  $\text{SrTiO}_3$  (FeSe/STO)[3] ( $T_c^{\text{max}}=65\text{K}$ , determined by angle-resolved photoemission spectroscopy (ARPES)[4]), stirred up a new wave of excitement in iron-based superconductors (FeSCs) research. In ARPES studies it is found, at ambient pressure, both systems have no hole pocket[4, 5]. Because it is often perceived that the scattering between the electron and hole pockets are important for both antiferromagnetism and Cooper pairing[6], this becomes an issue.

On a different front, recently many experimental evidences point to the fact that FeSCs have a tendency to become electronically “nematic”[7–9, 11, 12]. For example, through magnetic torque measurement Ref.[11] reported a phase diagram for  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$  where the superconducting dome is enclosed by a non-magnetic electronic nematic phase. In addition, Ref.[12] reported a divergent “nematic susceptibility” in  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$  close to the  $x$  value at which  $T_c^{\text{max}}$  occurs. In addition to these, an ARPES experiment by Yi *et al.*[9] established the tie between electronic nematicity and the  $d_{xz}$ ,  $d_{yz}$  orbital ordering. These experiments naturally raise the question: what role (if any) do orbital order or orbital fluctuation play in Cooper pairing?

The purpose of this paper is to address the above two questions. Our conclusions are summarized as follows. (1) Hole pockets introduce frustration in Cooper pairing (a concept we shall discuss later). To a large extent this is due to the existence of band vorticity around the hole fermi surface (see later). Removing the hole pockets releases pairing frustration, experimentally it is found this does not weaken the antiferromagnetic (AFM) correlation[13]. This makes Cooper pairing in  $A_x\text{Fe}_{2-y}\text{Se}_2$  and FeSe/STO stronger, hence higher  $T_c$ . Of course in FeSe/STO substrate screening can further enhance  $T_c$ [14]. (2) Orbital fluctuation has negligible effect on Cooper pairing while static orbital order can have large effect. (3) AFM fluctuation can still be the primary cause of Cooper pairing, but AFM is most likely due to local correlation not fermi surface nesting. (4) The inter-pocket hybridization tends to favor *in phase*

*s*-wave pairing in  $A_x\text{Fe}_{2-y}\text{Se}_2$  and FeSe/STO.

The above conclusions are reached by using an effective Hamiltonian approach. In this approach we write down a low energy Hamiltonian to capture the system’s tendencies toward (1) stripe antiferromagnetism[15–17] (2) superconducting pairing[18, 19], and (3)  $d_{xz}/d_{yz}$  orbital ordering[7–12]. The above tendencies are not only established experimentally, but also found theoretically[6, 20–23]. To a great extent, the derivation of the effective Hamiltonian has been achieved by the functional renormalization group (FRG) study in Ref.[25]. It’s conclusion has been checked by variational Monte-Carlo (VMC) calculation[26]. The last statement is significant because FeSCs are by no means weakly coupled systems[27].

Our effective Hamiltonian is given by:

$$H_{\text{eff}} = \sum_{\mathbf{k}, \alpha, \sigma} \epsilon_{\mathbf{k}\alpha} n_{\mathbf{k}\alpha\sigma} + \sum_{\mathbf{k}, \alpha, \sigma} \sum_{\mathbf{q}, \beta, \tau} F_{\mathbf{k}\alpha\sigma}^{\mathbf{q}\beta\tau} n_{\mathbf{k}\alpha\sigma} n_{\mathbf{q}\beta\tau} + \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + V \sum_i n_{i,xz} n_{i,yz}. \quad (1)$$

The first term is the bandstructure ( $\alpha, \beta$  = band indices,  $\sigma, \tau$  = spin indices). The second term is a multi-band version of the Fermi liquid interaction. In the third term  $\mathbf{S}_i = \frac{1}{2} \sum_a c_{i,a,s}^\dagger \vec{\sigma}_{ss'} c_{i,a,s'}$ , where  $a = d_{z^2}, d_{xz}, d_{yz}, d_{xy}, d_{x^2-y^2}$  is the orbital index. The last term of Eq. (1), with  $V > 0$ , describes the tendency toward the  $d_{xz}/d_{yz}$  orbital ordering[9, 23, 24]. We wrote the last two terms of Eq. (1) in real space, but they should be understood as been projected to the band eigen bases that lie in a thin shell around the fermi surface.

Eq. (1) describes several competing (or “intertwined”) instabilities, a hallmark of strongly correlated systems. Of course solving the effective Hamiltonian is a difficult problem. In the following we shall assume Cooper pairing is the winning instability, and our goal is simply to determine which pairing symmetry is favored the most. Some technical points: (1) In Eq. (1) we allowed the magnetic interaction to extend over arbitrary neighbors. However in Ref.[25] it has been shown if one retains only the first ( $J_1$ ) and second neighbor ( $J_2$ ) interaction, the effective Hamiltonian already qualitatively captures the numerical

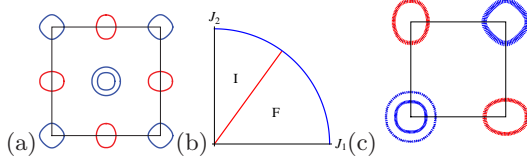


FIG. 1: (a) A caricature of the Fermi surface of Fe-pnictides. Here blue and red mark the hole and electron pockets, respectively. (b) The two regimes of pairing. The value of the critical angle (marked by the red line) is approximately  $0.3\pi$ . In the region marked “F” pairing is frustrated. (c) The typical gap function in region “I” of panel (b). The size is proportional to the magnitude and the color indicates the sign (blue: plus and red: minus). Only the first quadrant of the unfolded Brillouin zone is shown.

functional renormalization group results for the  $\mathbf{k}$  dependence of the AFM and SC order parameters. Since the purpose of this paper is to elucidate qualitative physics rather than providing quantitative predictions, we shall truncate  $J_{ij}$  to only  $J_1$  and  $J_2$ [28]. (2) Once the Fermi surface is fixed, the second term of Eq. (1) has no effect on Cooper pairing. Hence we shall drop it in the subsequent discussions. Finally on the semantics: when the various interaction in Eq. (1) fail to drive long range order, we call them “fluctuations”. For example the  $J_1, J_2$  terms will be termed “magnetic fluctuation”.

**Results for Fe-pnictide:** A plot of the typical Fermi surface for the Fe-pnictide systems is shown in Fig. 1(a), where both electron pocket (marked red) and hole-pocket (marked blue) are present. First we study the effect of magnetic interaction on pairing. We control the ratio between the AF  $J_1$  and  $J_2$  by introducing an angle  $\theta$

$$J_1 = J \cos \theta, \quad J_2 = J \sin \theta, \quad 0 \leq \theta \leq \pi/2. \quad (2)$$

We then project the effective Hamiltonian onto the singlet pairing channel to construct the following pairing “matrix”

$$M(\alpha, \phi; \beta, \phi') = U(\alpha, \phi; \beta, \phi') \frac{k_{F\beta}(\phi')}{v_{F\beta,r}(\phi')}. \quad (3)$$

Here  $U(\alpha, \phi; \beta, \phi')$  is the effective singlet pairing interaction on the Fermi surface ( $\alpha$  labels Fermi pockets and  $\phi$  is the angle around them),  $k_{F\beta}$  and  $v_{F\beta,r}$  are the magnitudes of the Fermi wavevector and the projection of the Fermi velocity along the radial direction, respectively. The leading gap function is the eigenfunction of  $M(\alpha, \phi; \beta, \phi')$  with the most negative eigenvalue. In case  $M(\alpha, \phi; \beta, \phi')$  has degenerate eigenvalues non-quadratic interaction terms between different superconducting order parameters are necessary to determine the pairing symmetry[29, 30]. In this paper we shall just focus on the quadratic instability. Depending on the value of  $\theta$ , there exists two pairing regimes marked by “I” and “F”

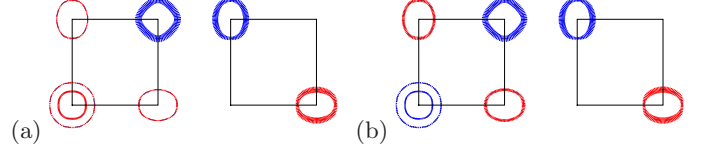


FIG. 2: The gap function in region “F” of Fig. 1(b). In the presence of the hole pockets (left panels in (a) and (b)) the gap function has s-wave symmetry and the sign of the gap function on the hole pockets changes as  $\theta$  increases from 0 (Fig.2(a)) to  $0.3\pi$  (Fig.2(b)). After removing the hole pockets (right panels in (a) and (b)) the symmetry becomes d-wave. Only the first quadrant of the unfolded Brillouin zone is shown.

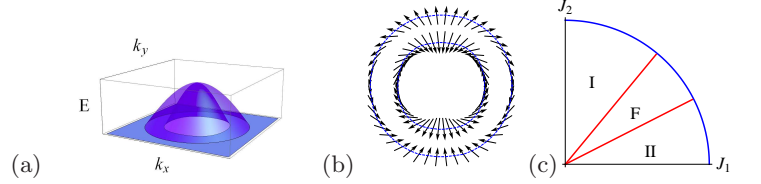


FIG. 3: The band vorticity associated with the hole pockets. (a) The band structure near  $\Gamma$ . (b) The pseudo spin winding (see text). (c) The region with pairing frustration substantially shrinks after the removal of the band vorticity of the hole Fermi surfaces. The values of the two critical angles (marked by the red lines) are approximately  $0.15\pi$  and  $0.28\pi$ . Only the first quadrant of the unfolded Brillouin zone is shown.

in Fig. 1(b). The representative gap functions in region I is shown in Fig. 1(c), it is  $\pm s$ . Cooper pairing in this region is *non-frustrated* in the sense that if we remove the hole pockets and recalculate the gap function on the electron pockets, the same sign structure is obtained.

In contrast, in region F pairing is frustrated. In Fig. 2(a,b) we show the gap function with and without the hole pockets in this region. Generally speaking the pairing symmetry is s-wave with hole pockets and d-wave without. The fact that after removing the hole pockets the symmetry of the gap function changes is reminiscent to the change of spin alignment from coplanar to collinear after removing a spin to unfrustrate the AF Heisenberg interaction on a triangle. In the literature[31] it is noted that there is a near degeneracy between the  $s_{\pm}$  and  $d_{x^2-y^2}$  pairing symmetry for values of the interaction parameters yielding significant pairing strength. We claim this degeneracy is due to the pairing frustration discussed above.

It turns out the pairing frustration is, to a large extent, caused by the band topology of the hole pockets. In Fig. 3(a) we show the dispersion of the hole bands near the center of the Brillouin zone. The double degeneracy at  $\Gamma$  is protected by the point group symmetry. A consequence of such degeneracy is the existence of “band vorticity” at  $\Gamma$  [32, 33]. To see that we first note the orbital content of the hole band eigenfunctions are pre-

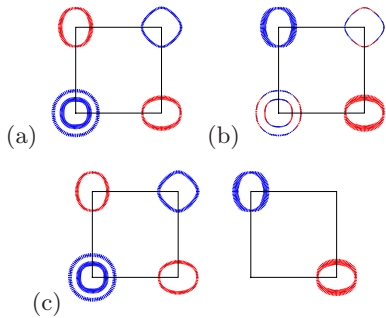


FIG. 4: (a) Typical gap function in region “I” of Fig. 3(c), there is no pairing frustration. (b) Typical gap function in region “II” of Fig. 3(c), there is no pairing frustration. (c) Typical gap function in region “F” of Fig. 3(c). There is pairing frustration. The left and right panels are the gap functions with and without the hole pockets. Only the first quadrant of the unfolded Brillouin zone is shown.

dominantly  $d_{xz}$  and  $d_{yz}$ . Let’s use a pseudo spin 1/2 to represent these two orbital states, e.g.,  $d_{xz} \rightarrow \tau_z = 1/2$  and  $d_{yz} \rightarrow \tau_z = -1/2$ . Using the band eigenfunctions we compute the expectation value of the pseudospin. The result lies in the x-z plane and the direction winds around the fermi surface (with vorticity 2) as shown in Fig. 3(b).

After we remove the hole band vorticity (by modifying the band wavefunction while maintaining the band dispersion) the frustrated pairing region substantially shrinks, as shown in Fig. 3(c). The typical gap function in region “I”, “II” and “F” are shown in Fig. 4(a,b,c). From this we conclude, the band vorticity associated with the hole pockets is an important cause of the pairing frustration. It is important to note, however, removing the band vorticity does not completely eliminate pairing frustration. What’s needed is the removal of the hole pockets entirely!

This motivates us to make the following conjecture: one reason that the absence of hole pockets raises  $T_c$  in  $A_x\text{Fe}_{2-y}\text{Se}_2$  and  $\text{FeSe}/\text{STO}$  is because the pairing frustration has been removed. However high  $T_c$  also requires strong AFM fluctuation (at least in the magnetic pairing scenario). If the AFM correlation is due to the nesting between the electron and hole fermi surfaces[6], one would predict the weakening of AFM fluctuation (hence the weakening of pairing). However the recent neutron scattering[13] experiment performed on “semiconducting”  $\text{K}_x\text{Fe}_{2-y}\text{Se}_2$  compounds neighboring the superconducting ones has revealed strong stripy AFM long range order peaking at the same wave vector as that observed in the parent pnictide compounds. This result suggests that it is better to view the AFM correlation in  $\text{FeSC}$  as due to local correlation physics, similar to the cuprates, instead of as coming from fermi surface nesting. More importantly it tells us the AFM fluctuation, needed for Cooper pairing, is strong in  $\text{K}_x\text{Fe}_{2-y}\text{Se}_2$  despite the ab-

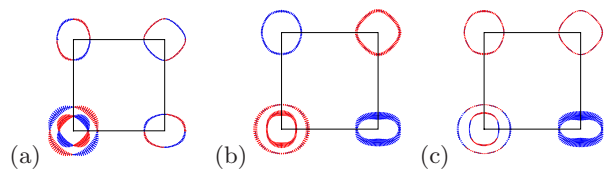


FIG. 5: (a) The gap function that is suppressed by the orbital fluctuation. (b,c) In the presence of static orbital ordering the frustration region also shrinks compared to Fig. 1(b). The phase diagram is qualitatively similar to Fig. 3(c) except the “F” region is slightly wider. The gap function in region “I” and “II” are shown in (b) and (c). Only the first quadrant of the unfolded Brillouin zone is shown.

sence of the hole pockets.

Motivated by Ref.[12] we next ask what is the effect of orbital fluctuation on Cooper pairing. To mimic orbital fluctuation we turn on the  $V$  term in Eq. (1). To our surprise, for all values of  $V$  this has no effect on pairing. To understand this result let us switch off  $J_1$  and  $J_2$  and look at the eigenfunctions of Eq. (3) when there is only the orbital interaction. It turns out in this case except one positive eigenvalue all other eigenvalues of  $M$  are zero. In Fig. 5(a) we illustrate the eigenfunction associated with the positive eigenvalue. Thus the orbital interaction lifts up the pairing eigenvalue associated the  $d_{xy}$  symmetry but leaves all other symmetry channels unaffected. In particular, this lifting does not affect the leading pairing symmetries, namely  $s$  and  $d_{x^2-y^2}$  in Fig. 1 and Fig. 2. The fact that  $V$  introduces only a single positive pairing eigenvalue is due to the on-site nature of the orbital interaction. Had we allowed for further neighbor orbital interaction, e.g.,  $V_0 \sum_i n_{i,xz} n_{i,yz} + V_1 \sum_{\langle ij \rangle} n_{i,xz} n_{j,yz}$  there will be more than one positive eigenvalues. For example if we choose  $V_1/V_0 = 0.5$  there are five positive eigenvalues (all other eigenvalues are still zero). Again, none of these five eigenfunctions has the symmetry of the leading pairing channel in Fig. 1 and Fig. 2. For all the cases we studied this is always true. Thus we conclude orbital fluctuation has no effect on pairing.

Because Ref.[11] claimed the superconducting dome in  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$  is embedded in a non-magnetic nematic phase, we next study the effect of static orbital order on pairing. In Fig. 5(b,c) we show the anisotropic gap function in the presence of a  $\delta E = 40$  meV energy splitting between the  $xz$  and  $yz$  orbitals, namely,  $\delta E \sum_i (n_{i,xz} - n_{i,yz})$ . If this anisotropy is observed by ARPES it will constitute a strong evidence for coexistence of superconductivity and nematic order.

**Results for the Fe-chalcogenide:** The fermiology of superconducting  $A_x\text{Fe}_{2-y}\text{Se}_2$  and  $\text{FeSe}/\text{STO}$  are rather similar - there are only electron pockets. As mentioned earlier due to the neutron scattering result of Ref.[13] there is every reason to believe the same magnetic in-

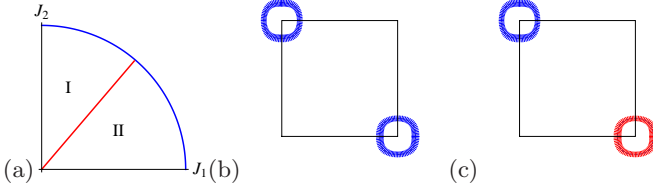


FIG. 6: Magnetic fluctuation induced pairing symmetry of systems with only electron Fermi surfaces. (a) Two different pairing regimes. The value of the critical angle (marked by the red line) is approximately  $0.27\pi$ . The gap function in region I (b) and II (c). Only the first quadrant of the unfolded Brillouin zone is shown.

interaction exists in the effective Hamiltonian (at least for  $K_x\text{Fe}_{2-y}\text{Se}_2$ ). Using bandstructures with only electron pockets[14, 34] our result for the gap function under different  $J_1$  and  $J_2$  ratio is shown in Fig. 6. Depending on whether  $J_1$  or  $J_2$  dominates, the pairing symmetry is either  $s$  wave or fully gapped  $d$ -wave, consistent with the findings in Ref.[35]. Interestingly despite the fact that AFM effective interaction is characteristic of a repulsive system, the in-phase  $s$ -wave pairing is found for a large region of parameter space.

Because nodeless  $d$ -wave occupies a significant region of parameter space in Fig. 6(a), it is important to investigate the effect of the electron pocket hybridization on the gap function. This hybridization exists (even for  $k_z = 0$ ) when the  $z \rightarrow -z$  glide plane symmetry is broken. For  $A_x\text{Fe}_{2-y}\text{Se}_2$  this occurs near the sample surface (which is what ARPES probes). For FeSe/STO there is no glide plane symmetry at all. It was first pointed out in Ref.[36] that when such hybridization is sufficiently strong it can modify the nodeless  $d$ -wave pairing state into nodal  $d$ -wave pairing.

In Fig. 7(a) we choose the hybridization matrix elements so that electron pockets are only slightly split and remain more or less circular. This choice is motivated by the fact that ARPES found rounded electron pocket without discernable splitting for both  $A_x\text{Fe}_{2-y}\text{Se}_2$ [5] and FeSe/STO[4].

In the presence of the electron pocket splitting, the phase diagram and gap function are shown in Fig. 7(b). The hybridization has clearly increased the range of stability for the  $s$ -wave pairing. Indeed there is a region of the phase diagram where the nodeless  $d$ -wave pairing has turned into a nodal one. However, the dominant pairing symmetry in Fig. 7(b) is the in-phase  $s$ -wave rather than the out-of-phase  $s$ -wave proposed in Ref.[36, 37]. This result is consistent with the recent ARPES result which rules out  $d$ -wave pairing based on the mapping of the gap function on the electron pockets center around  $\mathbf{k} = (0, 0, \pi)$ [38].

Finally we believe the substrate, namely  $\text{SrTiO}_3$ ,

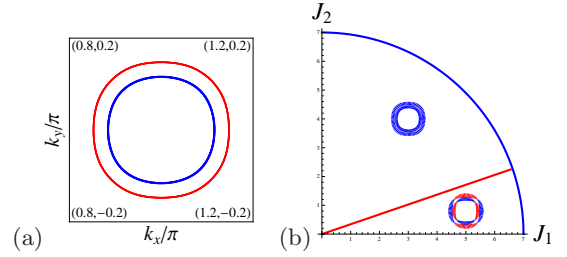


FIG. 7: (a) The hybridization-split electron pockets. (b) The gap function in the presence of hybridization. In panel (b) the splitting between the two electron Fermi surfaces has been enhanced to increase clarity. The value of the critical angle (marked by the red line) is approximately  $0.105\pi$ .

plays an important role in raising the  $T_c$  of FeSe/STO and further stabilize  $s$ -wave pairing. This is through the screening of the long range part of the Coulomb interaction[14]. As far as orbital fluctuation and orbital ordering are concerned, the results are very similar to those for systems with both electron and hole pockets.

**Conclusion:** We have used an effective Hamiltonian to address two important modern issues raised by the high  $T_c$   $A_x\text{Fe}_{2-y}\text{Se}_2$  and FeSe/STO superconductors. This effective Hamiltonian is constructed under the guidance of (1) FRG calculation[25], (2) VMC calculation[26] and (3) experiments[7–9, 11, 12, 15–19]. The issues are (1) the effect of fermiology on high temperature superconductivity and (2) the effects of orbital ordering and orbital fluctuations on Cooper pairing. Our conclusions are summarized in paragraph three of the introduction.

**Acknowledgments:** We Acknowledge Jun Zhao, Bob Birgeneau, Alessandra Lanzara and Qiang-hua Wang for helpful discussions. DHL acknowledges the support by the DOE grant number DE-AC02-05CH11231. FY is supported by the NSFC under the grant number 11274041, and the NCET program under the grant number NCET-12-0038.

- 
- [1] Jiangang Guo, Shifeng Jin, Gang Wang, Shunchong Wang, Kaixing Zhu, Tingting Zhou, Meng He, and Xiaolong Chen, Phys. Rev. B **82**, 180520(R) (2010).
  - [2] Liling Sun, Xiao-Jia Chen, Jing Guo, Peiwen Gao, Qing-Zhen Huang, Hangdong Wang, Minghu Fang, Xiaolong Chen, Genfu Chen, Qi Wu, Chao Zhang, Dachun Gu, Xiaoli Dong, Lin Wang, Ke Yang, Aiguo Li, Xi Dai, Hongkwang Mao, and Zhongxian Zhao, Nature **483**, 67 (2012).
  - [3] Qing-Yan Wang, Zhi Li, Wen-Hao Zhang, Zuo-Cheng Zhang, Jin-Song Zhang, Wei Li, Hao Ding, Yun-Bo Ou, Peng Deng, Kai Chang, Jing Wen, Can-Li Song, Ke He, Jin-Feng Jia, Shuai-Hua Ji, Ya-Yu Wang, Li-Li Wang, Xi Chen, Xu-Cun Ma, and Qi-Kun Xue, Chin. Phys. Lett.



- 29**, 037402 (2012).
- [4] Defa Liu, Wenhao Zhang, Daixiang Mou, Junfeng He, Yun-Bo Ou, Qing-Yan Wang, Zhi Li, Lili Wang, Lin Zhao, Shaolong He, Yingying Peng, Xu Liu, Chaoyu Chen, Li Yu, Guodong Liu, Xiaoli Dong, Jun Zhang, Chuangtian Chen, Zuyan Xu, Jiangping Hu, Xi Chen, Xucun Ma, Qikun Xue, and X.J. Zhou, *Nature Commun.* **3**, 931 (2012).
  - [5] Y. Zhang, L. X. Yang, M. Xu, Z. R. Ye, F. Chen, C. He, H. C. Xu, J. Jiang, B. P. Xie, J. J. Ying, X. F. Wang, X. H. Chen, J. P. Hu, M. Matsunami, S. Kimura, and D. L. Feng, *Nat. Mater.* **10**, 273 (2011).
  - [6] I. I. Mazin, D. J. Singh, M. D. Johannes, and M. H. Du, *Phys. Rev. Lett.* **101**, 057003 (2008).
  - [7] T.-M. Chuang, M. P. Allan, Jinho Lee, Yang Xie, Ni Ni, S. L. Budko, G. S. Boebinger, P. C. Canfield, and J. C. Davis, *Science* **327**, 181 (2010).
  - [8] Jiun-Haw Chu, James G. Analytis, Kristiaan De Greve, Peter L. McMahon, Zahirul Islam, Yoshihisa Yamamoto, and Ian R. Fisher, *Science* **329**, 824 (2010).
  - [9] Ming Yi, Donghui Lu, Jiun-Haw Chu, James G. Analytis, Adam P. Sorini, Alexander F. Kemper, Brian Moritz, Sung-Kwan Mo, Rob G. Moore, Makoto Hashimoto, Wei-Sheng Lee, Zahid Hussain, Thomas P. Devereaux, Ian R. Fisher, and Zhi-Xun Shen, *PNAS* **108**, 6878 (2011).
  - [10] Can-Li Song, Yi-Lin Wang, Peng Cheng, Ye-Ping Jiang, Wei Li, Tong Zhang, Zhi Li, Ke He, Lili Wang, Jin-Feng Jia, Hsiang-Hsuan Hung, Congjun Wu, Xucun Ma, Xi Chen, and Qi-Kun Xue, *Science* **332**, 1410 (2011).
  - [11] S. Kasahara, H. J. Shi, K. Hashimoto, S. Tonegawa, Y. Mizukami, T. Shibauchi, K. Sugimoto, T. Fukuda, T. Terashima, Andriy H. Nevidomskyy, and Y. Matsuda, *Nature*, **486**, 382 (2012).
  - [12] Jiun-Haw Chu, Hsueh-Hui Kuo, James G. Analytis, and Ian R. Fisher, *Science* **337**, 710 (2012).
  - [13] J. Zhao, H. Cao, E. Bourret-Courchesne, D. -H. Lee, and R. J. Birgeneau, *Phys. Rev. Lett.* **109**, 267003 (2012).
  - [14] Y.-Y. Xiang, F. Wang, D. Wang, Q.-H. Wang, and D.-H. Lee, *Phys. Rev. B* **86**, 134508 (2012).
  - [15] Clarina de la Cruz, Q. Huang, J. W. Lynn, Jiying Li, W. Ratcliff II, J. L. Zarestky, H. A. Mook, G. F. Chen, J. L. Luo, N. L. Wang, and Pengcheng Dai, *Nature* **453**, 899 (2008).
  - [16] Q. Huang, Y. Qiu, Wei Bao, M. A. Green, J. W. Lynn, Y. C. Gasparovic, T. Wu, G. Wu, and X. H. Chen, *Phys. Rev. Lett.* **101**, 257003 (2008).
  - [17] Jun Zhao, Q. Huang, Clarina de la Cruz, Shiliang Li, J. W. Lynn, Y. Chen, M. A. Green, G. F. Chen, G. Li, Z. Li, J. L. Luo, N. L. Wang, and Pengcheng Dai, *Nat. Mater.* **7**, 953 (2008).
  - [18] Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, *J. Am. Chem. Soc.* **130**, 3296 (2008).
  - [19] Ren Zhi-An, Lu Wei, Yang Jie, Yi Wei, Shen Xiao-Li, Zheng-Cai, Che Guang-Can, Dong Xiao-Li, Sun Li-Ling, Zhou Fang, and Zhao Zhong-Xian, *Chin. Phys. Lett.* **25**, 2215 (2008).
  - [20] J. Dong, H. J. Zhang, G. Xu, Z. Li, G. Li, W. Z. Hu, D. Wu, G. F. Chen, X. Dai, J. L. Luo, Z. Fang, and N. L. Wang, *Europhys. Lett.* **83**, 27006 (2008).
  - [21] Kazuhiko Kuroki, Seiichiro Onari, Ryotaro Arita, Hidetomo Usui, Yukio Tanaka, Hiroshi Kontani, and Hideo Aoki, *Phys. Rev. Lett.* **101**, 087004 (2008).
  - [22] F. Wang, H. Zhai, Y. Ran, A. Vishwanath, and D.-H. Lee, *Phys. Rev. Lett.* **102**, 047005 (2009).
  - [23] C.-C. Lee, W.-G. Yin, and W. Ku, *Phys. Rev. Lett.* **103**, 267001 (2009).
  - [24] Weicheng Lv, Jiansheng Wu, and Philip Phillips, *Phys. Rev. B* **80**, 224506 (2009).
  - [25] H. Zhai, F. Wang, and D.-H. Lee, *Phys. Rev. B* **80**, 064517 (2009).
  - [26] F. Yang, H. Zhai, F. Wang, and D.-H. Lee, *Phys. Rev. B* **83**, 134502 (2011).
  - [27] M. M. Qazilbash, J. J. Hamlin, R. E. Baumbach, Lijun Zhang, D. J. Singh, M. B. Maple, and D. N. Basov, *Nature Physics* **5**, 647 (2009).
  - [28] K. Seo, B. A. Bernevig, and J. P. Hu, *Phys. Rev. Lett.* **101**, 206404 (2008).
  - [29] W.-C. Lee, S.-C. Zhang, and C. Wu, *Phys. Rev. Lett.* **102**, 217002 (2009).
  - [30] V. Stanev, and Z. Tesanovic, *Phys. Rev. B* **81**, 134522 (2010).
  - [31] S. Graser, T. A. Maier, P. J. Hirschfeld, and D. J. Scalapino, *New Journal of Physics* **11**, 025016 (2009).
  - [32] X.-L. Qi, S. Raghu, C.-X. Liu, D. J. Scalapino, and S.-C. Zhang, *arXiv:0804.4332* (unpublished).
  - [33] Y. Ran, F. Wang, H. Zhai, A. Vishwanath, and D.-H. Lee, *Phys. Rev. B* **79**, 014505 (2009).
  - [34] F. Wang, F. Yang, M. Gao, Z.-Y. Lu, T. Xiang, and D.-H. Lee, *Europhys. Lett.* **93**, 57003 (2011).
  - [35] Chen Fang, Yang-Le Wu, Ronny Thomale, B. Andrei Bernevig, and Jiangping Hu, *Phys. Rev. X* **1**, 011009 (2011).
  - [36] I. I. Mazin, *Phys. Rev. B* **84**, 024529 (2011).
  - [37] M. Khodas, and A. V. Chubukov, *Phys. Rev. Lett.* **108**, 247003 (2012).
  - [38] M. Xu, Q. Q. Ge, R. Peng, Z. R. Ye, Juan Jiang, F. Chen, X. P. Shen, B. P. Xie, Y. Zhang, A. F. Wang, X. F. Wang, X. H. Chen, and D. L. Feng, *Phys. Rev. B* **85**, 220504 (2012).